Elongated Fermi superfluid: absence of critical imbalance enhancement at equilibrium

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We show that the maximum population imbalance ratio $P_{\rm CC}$ for a two-component Fermi gas near the unitarity limit to condense does not increase with the trap aspect ratio λ, by two methods of 1) solving the Bogoliubov-de Gennes equations with coupling-constant renormalization, and 2) studying the pairing susceptibility by the real-space self-consistent T-matrix approximation. The deviation of the cloud shape from what is expected from the trap shape increases but stays minor with increasing λ up to 50. This finding indicates that despite the apparent discrepancy between the MIT and Rice experiments over the value of $P_{\rm CC}$ and the validity of local density approximation, the equilibrium state of the system for the aspect ratio in the Rice experiment should be consistent with that of MIT.

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Gaseous Fermi superfluids are endowed with new degrees of controllability over population difference and trap anisotropy. Imbalanced superfluidity of ^{6}Li has been observed by the Rice [1] and MIT [2] groups, but their results have shown marked differences over the validity of local density approximation (LDA) and the Chandrasekhar-Clogston (CC) limit – the upper bound $P_{\rm CC}$ of imbalance parameter $P \equiv (N_\uparrow - N_\downarrow)/N$ beyond which superfluidity breaks down [3], where $N_\uparrow$ and $N_\downarrow$ are the numbers of majority and minority atoms, and $N \equiv N_\uparrow + N_\downarrow$ is the total atom number. In the MIT experiment the profiles of both majority and minority clouds obey LDA, while in the Rice experiment with a very elongated trap and fewer atoms, LDA apparently breaks down. The CC limit was observed at MIT but not at Rice. A phenomenological surface tension [4, 5] of the condensate was shown to reproduce the deformation observed by the Rice group, but how to reconcile the apparently contradicting experimental differences without free parameters remains elusive [6, 7]. More recently the non-equilibrium state during the evaporative cooling process [8] was discussed to explain the Rice results. In this Letter we demonstrate, for the equilibrium state of the system at low and finite temperatures, that 1) the CC limit does not increase with increasing the trap aspect ratio λ, and that 2) while the density-difference distribution does deform from what is expected from the trap shape, the deformation is not as significant as in the Rice experiment for the number of atoms as small as 3×10^4.

We consider a system of atoms with mass m confined in an axisymmetric harmonic potential $V(\mathbf{r}) \equiv m(\omega_\perp^2(x^2+y^2)+\omega_z^2 z^2)/2$ with axial frequency ω_z and radial one $\omega_\perp$, and analyze superfluidity of this system using the Bogoliubov-de Gennes (BdG) equations [9–16]. Sensarma *et al.* [15] studied the shape of the atom cloud by changing N and $P(\leq 0.4)$, and argued that $(N/\lambda)^{1/3} \gg 1$ ($\lambda \equiv \omega_\perp/\omega_z$) should be the condition for the validity of LDA. For $(N/\lambda)^{1/3} \sim 10$, the cloud shape obtained in Ref. [15] looks quite similar to that of the equipotential surface. However, the Rice experiment shows the breakdown of LDA for almost the same value of $(N/\lambda)^{1/3}$. While our numerical results also show deformation similar to that found in Ref. [15] for $N \sim 10^3$ at $\lambda = 4$, the density profiles are different presumably because we incorporate the effect of the chemical potential difference as well as the interaction between atoms in the normal state. Such deformation almost disappears for $N \sim 3 \times 10^4$.

The BdG equations for unequal chemical potentials $(\mu_\uparrow, \mu_\downarrow)$ are given by

$$\begin{pmatrix} \hat{H}_\uparrow + W_\downarrow & \Delta \\ \Delta^* & -\hat{H}_\downarrow - W_\uparrow \end{pmatrix} \begin{pmatrix} u_q \\ v_q \end{pmatrix} = \epsilon_q \begin{pmatrix} u_q \\ v_q \end{pmatrix}, \quad (1)$$

where $\hat{H}_\sigma \equiv -\boldsymbol{\nabla}^2/(2m) + V(\boldsymbol{r}) - \mu_\sigma$ ($\sigma = \uparrow, \downarrow$) is the one-body Hamiltonian, and $W_\sigma(\boldsymbol{r})$ is the Hartree-Fock mean-field energy $g n_\sigma(\boldsymbol{r})$ with the coupling constant g given in terms of s-wave scattering length a_s as $g = 4\pi\hbar^2 a_s/m$. In the following we take $m = \hbar = k_{\rm B} = 1$, set $\overline{\omega} \equiv \sqrt[3]{\omega_\perp^2 \omega_z} = \omega_\perp/\sqrt[3]{\lambda}$, and choose $\sqrt{\hbar/(m\overline{\omega})} = 1$ as the unit of length. The self-consistent conditions give the density distributions $n_\sigma(\boldsymbol{r})$ and the s-wave singlet pair amplitude $\Delta(\boldsymbol{r})$ as

$$n_\uparrow(\boldsymbol{r}) = \sum_q f_q |u_q(\boldsymbol{r})|^2, n_\downarrow(\boldsymbol{r}) = \sum_q (1-f_q)\,|v_q(\boldsymbol{r})|^2,$$
$$\Delta(\boldsymbol{r}) = g_{\rm eff}(\boldsymbol{r}) \sum_q f_q u_q(\boldsymbol{r}) v_q^*(\boldsymbol{r}), \quad (2)$$

where $f_q \equiv (e^{\beta\epsilon_q}+1)^{-1}$ is the Fermi distribution function with $\beta \equiv (k_{\rm B}T)^{-1}$. To cope with the ultraviolet divergence in $\Delta(\boldsymbol{r})$, we follow Bulgac and Yu [17] and treat the contribution from states above an energy cutoff E_c within LDA. In Ref. [17], where $\mu = \mu_\uparrow = \mu_\downarrow$ is assumed, the single-particle Green's function G_μ^0 with $\hat{H}_0 = -\boldsymbol{\nabla}^2/(2m) + V - \mu$ is used to remove the divergence. The regular part $G_\mu^{0,\rm reg}$ of G_μ^0 is obtained by employing the Thomas-Fermi approximation for the states above E_c, so that the effective coupling constant is given in terms of $k_{\rm c}(\boldsymbol{r}) \equiv \sqrt{2\,(E_c - V(\boldsymbol{r}))}$ and $k_{\rm F}^0(\boldsymbol{r}) \equiv$

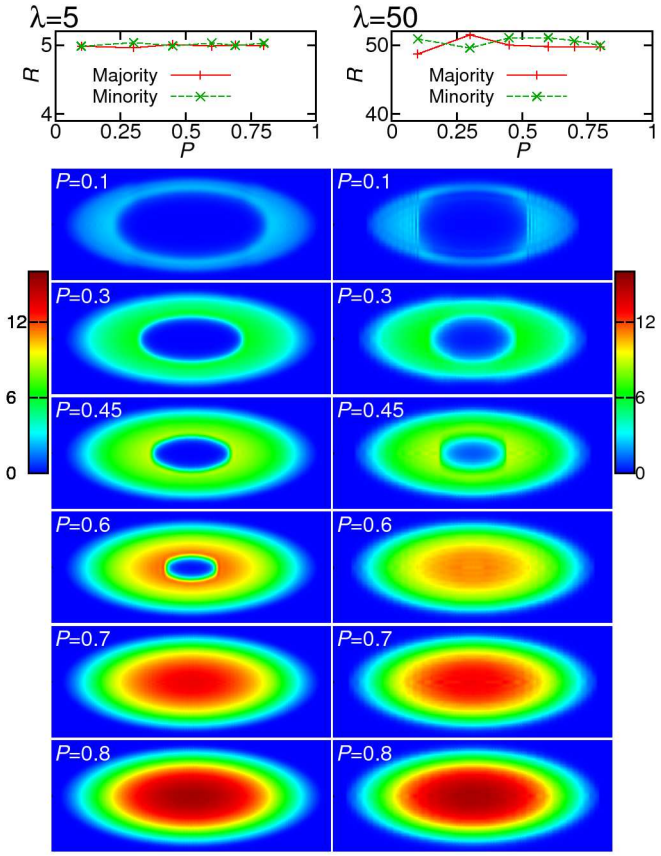

FIG. 1. (Color online) Top panel shows the P dependence of the ratio R of the axial to radial cloud widths at which the atomic density equals $1/20$ of its peak value. Lower panels show the density difference between majority and minority atoms plotted for $\lambda = 5$ (left) and 50 (right) with $k_{\rm F}a_s = -1.3$, $N = 3 \times 10^4$, and varying imbalance parameter P. The trap axis lies in the horizontal direction. At $\lambda = 5$, $(\mu_\uparrow, \mu_\downarrow) = (38.83, 28.80)$ for $P = 0.1$ and $(53.08, 4.79)$ for $P = 0.8$; at $\lambda = 50$, $(\mu_\uparrow, \mu_\downarrow) = (38.63, 28.78)$ for $P = 0.1$ and $(53.13, 4.66)$ for $P = 0.8$.

$\sqrt{2\left(\mu - V(\boldsymbol{r})\right)}$ as

$$\frac{1}{g_{\rm eff}(\boldsymbol{r})} = \frac{1}{g} + \frac{1}{2\pi^2}\left(\frac{k_{\rm F}^0(\boldsymbol{r})}{2}\ln\frac{k_{\rm c}(\boldsymbol{r}) + k_{\rm F}^0(\boldsymbol{r})}{k_{\rm c}(\boldsymbol{r}) - k_{\rm F}^0(\boldsymbol{r})} - k_{\rm c}(\boldsymbol{r})\right). \quad (3)$$

Grasso and Urban [18] replaced $k_{\rm F}^0(\boldsymbol{r})$ with $\tilde{k}_{\rm F}(\boldsymbol{r}) \equiv \sqrt{2\left(\mu - V(\boldsymbol{r}) - W(\boldsymbol{r})\right)}$, where $W(\boldsymbol{r}) = W_{\uparrow,\downarrow}$ for $\mu_\uparrow = \mu_\downarrow$, so that the convergence is achieved for much smaller values of E_c. We adopt this method except that we replace $G_\mu^{0,\rm reg}$ by $\left(G_{\mu_\uparrow}^{0,\rm reg} + G_{\mu_\downarrow}^{0,\rm reg}\right)/2$ to maintain a given chemical potential difference. Consequently, Eq. (3) is replaced by

$$\frac{1}{g_{\rm eff}(\boldsymbol{r})} = \frac{1}{g} + \frac{1}{2\pi^2}\left(\sum_\sigma \frac{\tilde{k}_{{\rm F}\sigma}}{4}\ln\frac{k_{\rm c} + \tilde{k}_{{\rm F}\sigma}}{k_{\rm c} - \tilde{k}_{{\rm F}\sigma}} - k_{\rm c}\right), \quad (4)$$

where $\tilde{k}_{{\rm F}\sigma}(\boldsymbol{r}) \equiv \sqrt{2\left(\mu_\sigma - V(\boldsymbol{r}) - W_{\overline{\sigma}}(\boldsymbol{r})\right)}$, with $W_\sigma(\boldsymbol{r}) = g n_\sigma(\boldsymbol{r})$. While BdG theory was originally proposed to describe the weak-coupling BCS limit, it was demonstrated to describe the BEC limit [19], and the BCS-BEC crossover region was also studied by this theory [20]. We therefore expect that this theory is applicable, at least qualitatively, for the strongly interacting region with population imbalance, provided that an appropriate coupling-constant renormalization is employed.

At the unitarity limit $(k_{\rm F}a_s)^{-1} \to 0$, the normal state interaction does not diverge, and the binding energy of a single $\downarrow$ atom to the Fermi sea of $\uparrow$ atoms with the Fermi energy $E_{{\rm F}\uparrow}$ is $-(3/5)AE_{{\rm F}\uparrow}$ with $A = 0.97(2)$ [21]. This corresponds to the mean-field energy of $-(9A\pi/20)\left(k_{{\rm F}\uparrow}(\boldsymbol{r})\right)^{-1} \times 4\pi n_\uparrow(\boldsymbol{r}) n_\downarrow(\boldsymbol{r})$, where $k_{{\rm F}\sigma} \equiv (6\pi^2 n_\sigma)^{1/3}$. On the BCS side of the unitarity limit, the normal state interaction should be weaker than at the unitarity limit so $|k_{{\rm F}\uparrow}(\boldsymbol{r})a_s| \le |k_{\rm F}(\boldsymbol{0})a_s| < 9A\pi/20 = 1.37$. Moreover, we can show that the BdG equations (1) do not have a stable self-consistent solution for $|k_{\rm F}a_s| > 3\pi/4 = 2.36$ for the homogeneous case without chemical potential difference.

We take $k_{\rm B}T = 0.05\hbar\overline{\omega}$ and use the Steffensen iteration to solve Eqs. (1) and (2), to self-consistently determine $n_\uparrow(\boldsymbol{r})$, $n_\downarrow(\boldsymbol{r})$ and $\Delta(\boldsymbol{r})$ for a given set of $(\mu_\uparrow, \mu_\downarrow)$. The number of atoms in the $\sigma(=\uparrow,\downarrow)$ state is defined as $N_\sigma \equiv \int {\rm d}^3 r n_\sigma$.

Figure 1 shows the main results of this Letter. For both $\lambda = 5$ and $\lambda = 50$, the ratio of the axial to radial cloud widths remains close to λ for both minority and majority atoms, and the dip of the density difference rapidly dwindles with increasing P, vanishing for $P > 0.75$. Thus the CC limit is not enhanced as λ is increased. For $\lambda = 50$, the density difference shows some deformation for small P, but it disappears for $P \gtrsim 0.60$.

Figure 2 shows typical distributions of $n_{\uparrow,\downarrow}$, their difference, and Δ for $P = 0.40$. We rescale the calculated distribution as $r \to \lambda r$ so that the equipotential surface becomes a circle. For $\lambda = 5$, the shape of the minority component and the density difference closely follow the equipotential surface, as shown in the left column of Fig. 1. The pair amplitude shows sign changes, which are absent in LDA but shows up in the BdG simulation as discussed in Ref. [13] for a spherical system.

For P larger than 0.7, the pair amplitude almost vanishes, and the density difference peaks at $\boldsymbol{r} = \boldsymbol{0}$. We therefore conclude that LDA is essentially valid at $\lambda = 5$ as observed by the MIT group. For $\lambda = 50$, while the density difference shows some deviation from the trap shape, implying the breakdown of LDA, the degree of breakdown is rather small. This can be seen from almost spherical density distributions of both the majority and minority components in Fig. 2. (Note that in Fig. 2 the vertical axis is scaled by a factor of λ.) The region with non-vanishing pairing amplitude is also rather similar to that of the minority component, reflecting the fact that pairing occurs effectively in the strongly interacting regime.

With the same number of atoms, we have thus confirmed that LDA is less invalid at $\lambda = 5$ than at $\lambda = 50$. The breakdown of LDA is a finite-size effect, and it is enhanced for larger λ. Figure 3 shows the atom-number dependence of $P_{\rm CC}$ for a spherical trap. We find that with increasing N,

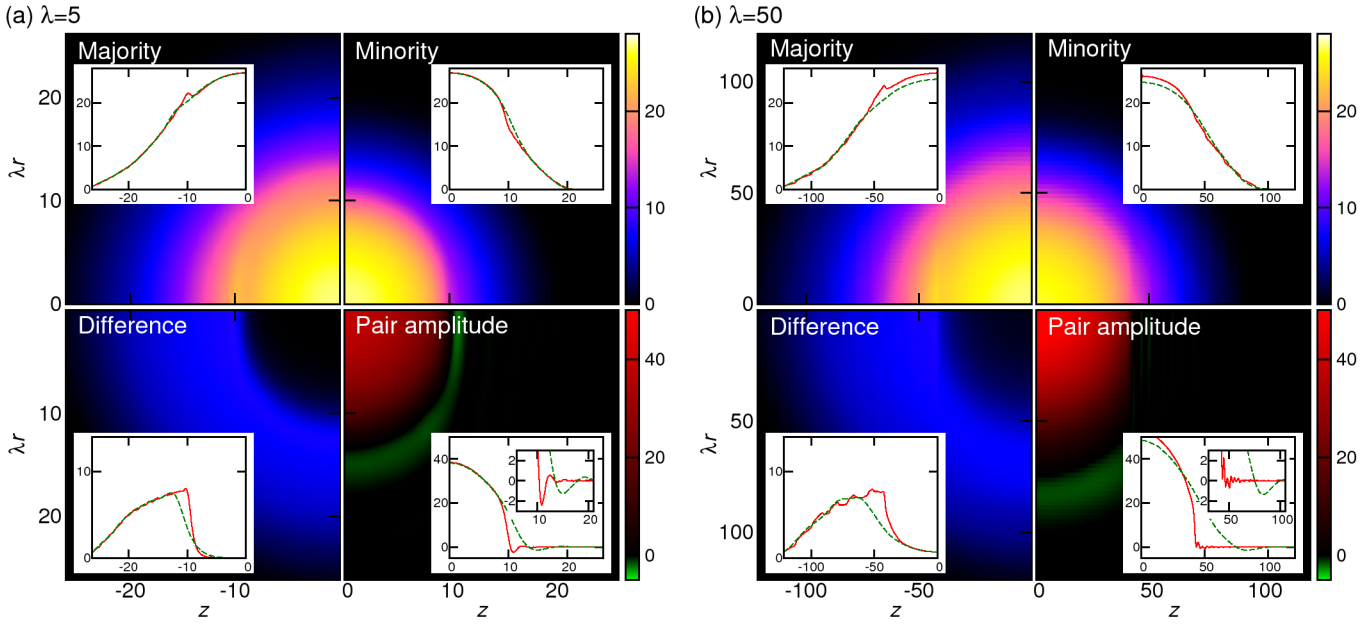

FIG. 2. (Color online) Majority and minority density distributions $n_{\uparrow,\downarrow}(z,r)$, their difference $n_\uparrow(z,r)-n_\downarrow(z,r)$ and pair amplitude $\Delta(z,r)$ plotted for (a) $\lambda=5$ and (b) $\lambda=50$ with $k_{\mathrm{F}\uparrow}a_s=-1.3$ and $N=3\times10^4$ at $P=0.40$. $(\mu_\uparrow,\mu_\downarrow)=(45.90,19.20)$ in (a) and $(45.57,19.42)$ in (b). The density distributions and Δ are displayed in color-coded gauges shown on the upper right and lower right, respectively. In each inset, the cross sections at $r=0$ (solid curve) and $z=0$ (dashed curve) are plotted against z and λr, respectively. For the pair amplitude, the regions close to the horizontal axis are enlarged in the smaller insets.

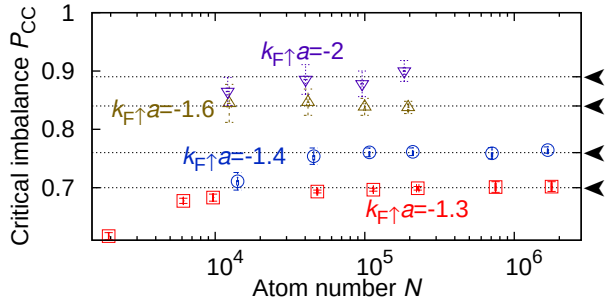

FIG. 3. (Color online) CC limit P_{CC} plotted against the total number of trapped atoms N in a spherical harmonic potential. Here, P_{CC} is identified as the value of P at which the extrapolated plot of $\Delta(\mathbf{0})$ crosses zero.

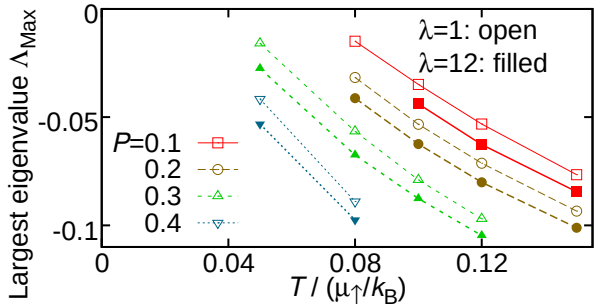

FIG. 4. (Color online) Largest eigenvalue Λ_{Max} of χ_{SC} obtained in the RSTA method is plotted against $T/(\mu_\uparrow/k_{\mathrm{B}})$ for $\mu_\uparrow=10\hbar\overline{\omega}=10\hbar\sqrt[3]{\omega_z\omega_r^2}$ for aspect ratios $\lambda=1$ (open symbols) and 12 (filled) and imbalance parameters $P=0.1,0.2,0.3,0.4$.

P_{CC} approaches a constant value for each $|k_{\mathrm{F}\uparrow}a_s|$, which is, for $|k_{\mathrm{F}\uparrow}a_s|=1.3$, close to the value at which the pair amplitude disappears in the elongated traps with $\lambda=5$ and 50.

To show that the non-increasing behavior of P_{CC} for increasing λ is not an artifact of the BdG approximation or a finite $k_{\mathrm{F}\uparrow}a_s$, we employ the real-space self-consistent T-matrix approximation [22] (RSTA), by which strongly interacting fermions in an inhomogeneous potential can be treated with high accuracy. RSTA has been shown to reproduce the pseudo-gap phase in high-T_{c} superconductors [22] and the superconductor-insulator transition in disordered diamond superconductors [23].

At the unitarity limit $(1/(k_{\mathrm{F}}a_s)\to0)$, in the normal phase we self-consistently solve the following set of equations:

$$\chi_{\mathrm{SC}}(\boldsymbol{r},\boldsymbol{r}')=T\sum_n G_\uparrow(\boldsymbol{r},\boldsymbol{r}',\omega_n)G_\downarrow(\boldsymbol{r},\boldsymbol{r}',-\omega_n) - C(\boldsymbol{r})\delta(\boldsymbol{r},\boldsymbol{r}'), \tag{5}$$

$$\tilde{T}(\boldsymbol{r},\boldsymbol{r}')=\left[g^{-1}\delta(\boldsymbol{r},\boldsymbol{r}')+\chi_{\mathrm{SC}}(\boldsymbol{r},\boldsymbol{r}')\right]^{-1}, \tag{6}$$

$$\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}',\omega_n)=TG_{\overline{\sigma}}(\boldsymbol{r}',\boldsymbol{r},-\omega_n)\tilde{T}(\boldsymbol{r},\boldsymbol{r}'), \tag{7}$$

$$G_\sigma(\boldsymbol{r},\boldsymbol{r}',\omega_n)=\left[\left[G^0_\sigma(\boldsymbol{r},\boldsymbol{r}',\omega_n)\right]^{-1}-\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}',\omega_n)\right]^{-1} \tag{8}$$

where χ_{SC} is the pairing susceptibility, G_σ (G^0_σ) the (non-interacting) Green's function, Σ_σ the self-energy, ω_n =

$(2n+1)\pi/T$ the Matsubara frequencies, and $C(\boldsymbol{r})$ the space-dependent regularization factor, which is obtained as

$$C(\boldsymbol{r};\omega_{\rm c};E_{\rm Max}) = \pi^{-3}\int_0^{\sqrt{2(E_{\rm Max}-V(\boldsymbol{r}))}} \arctan\left(\frac{2\omega_{\rm c}}{k^2}\right)\mathrm{d}k. \tag{9}$$

We discretize the system and use the rotational symmetry of the system to use a Fourier component expression in the relative azimuthal angle between two spatial lattice points. We need about 15 (positive) Matsubara frequencies, $E_{\rm Max}\sim 30\hbar\overline{\omega}$ and $30-60$ Fourier components for convergence at $\mu_\uparrow = 10\hbar\overline{\omega} \geq \mu_\downarrow$ and $\lambda = 1$ or 12.

If the phase transition from a normal gas to a superfluid is due to the divergence of the T-matrix, the maximum eigenvalue $\Lambda_{\rm Max}$ of $\chi_{\rm SC}$ reaches zero from below at the transition point $T_{\rm c}$. While in our trapped, finite-size system a first-order transition may occur, and then $\Lambda_{\rm Max}$ is not necessarily zero, we believe that the transition should happen at similar values of $\Lambda_{\rm Max}$ close to zero regardless of the trap aspect ratio λ if the total number N and temperature T are similar. Therefore, we compare $\Lambda_{\rm Max}$ as a function of $\mu_\downarrow$ for a fixed $\mu_\uparrow$ and T.

As shown in Fig. 4, for $\lambda = 12$, the value of $\Lambda_{\rm Max}$ is close to, but does not exceed, that for $\lambda = 1$. This comparison is for aspect ratios smaller than those of MIT and Rice; however, because the effects of the trap shape are enhanced for smaller N, this result indicates that in the equilibrium, for $N \gg 10^4$ atoms, the transition temperatures for a given P for $\lambda = 50$ should not exceed that for $\lambda = 5$, and strengthens our conclusion that $P_{\rm CC}$ is not enhanced as λ is increased.

To summarize, we have studied superfluidity of population-imbalanced fermions trapped in an axisymmetric harmonic trap by means of the Bogoliubov-de Gennes method. Our numerical results reproduce the major features of the experiments conducted at MIT, but does not reproduce those at Rice, as to the value of $P_{\rm CC}$ and as to the degree of LDA breakdown. Recently Nascimbène and coworkers at ENS Paris [24] have trapped population-imbalanced fermions in elongated traps with various values of the aspect ratio and observed $P_{\rm CC} = 0.76(3)$ and no deformation of density profiles. Zwierlein and coworkers at MIT [25] observed very long spin diffusion time in two-species fermionic gases at unitarity by making two polarized gases collide in a quasi one-dimensional potential. The diffusion constant extracted from their experiment suggests that the timescale of the equilibration is as long as one second for the configuration of the Rice experiment, which is much longer than the waiting time after the potential ramp in that experiment. We speculate that in the Rice experiment for $P > 0.8$, a non-equilibrium condensate state, possibly from the mechanism discussed in [8], was observed in the course of slow relaxation and cooling process into a normal state.

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